CHAPTER 2 THEORY AND LITURATURE REVIEWS

In this chapter, the theory and literature review are presented give the general comprehension and knowledge related to this thesis. The theories can be divided into 7 sections. First, the fundamental of plastic injection molding process, which consists of 3 stages namely filling, cooling and ejection stages, is explained. Then, the variables of filling stage of injection molding process showing effects on the stability of plastic parts are shortly concluded. Next, the rheology of the selected material, PLA, is discussed including the basic information about plastic flow characteristic. Moreover, the computational fluid dynamics (CFD) including mesh topologies are presented. The relevant literature reviews are shown in last section.

2.1 The plastic injection molding process [5, 6]

Injection molding is the most widely used method in manufacturing process for the fabrication of plastic parts. Because the injection molding can handle the complexity of shape and it also gives the accuracy in dimensions. This method requires the use of an injection molding machine, raw plastic material, and a mold which are shown in Figure 2.1. The cycle of injection molding is very short- regularly between 2 seconds to 2 minutes.

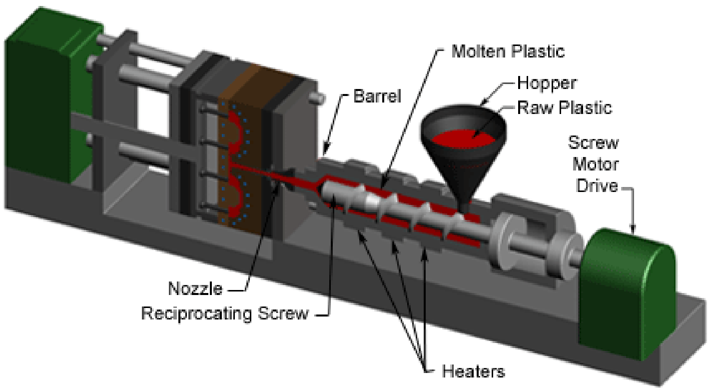

Figure 2.1 Injection molding machine [6]

There are 3 main stages which consist of filling, cooling and ejection stages respectively. The details of all stages are shown as follows.

2.1.1 Filling stage

The pellet plastics are used as raw material which are fed into the injection molding machine and sent towards the mold by the injection part. During this process, the material is melted by heat. Then, the melted plastic is speedily shot into the mold cavity and the pressure is built to pack and hold the material (see Figure 2.2).

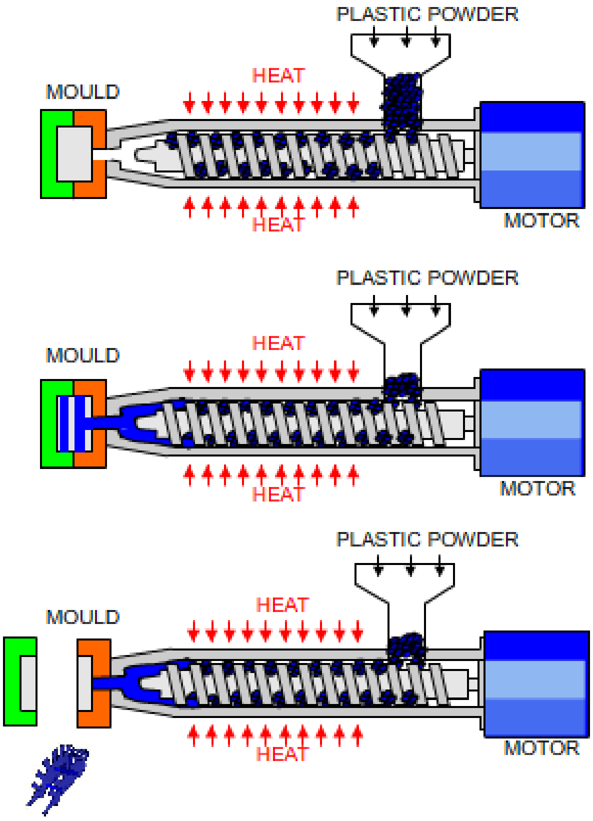

Figure 2.2 Injection molding process [5]

2.1.2 Cooling stage

The molten plastic that is inside the mold starts to cool down until it attaches with the inner mold surfaces. While the plastic cools, it will solidify into the desired shape of mold. However, during cooling some shrinkage and warpage of the part may happen. The mold will not be opened until the required cooling time has passed.

2.1.3 Ejection stage

After enough time has passed, the cooled part will be ejected from the mold by the ejection system. When the mold is opened, a mechanism is used to push the part out of the mold. In order to push the solidified part out of mold, the external force has to be applied because pending cooling the surface of plastic part sticks and shrinks to the inner mold surface. However, the release agent spray may be sprayed onto the surfaces of mold before filling stage to take plastic part out of mold easier.

2.2 The injection molding parameters [4]

After the injection molding process is finished, the equality of final product must be investigated in terms of appearance, dimension and mechanical properties. Definitely the low quality of plastic product may occur due to inappropriate the injection molding parameters, which are expressed in Figure 2.3.

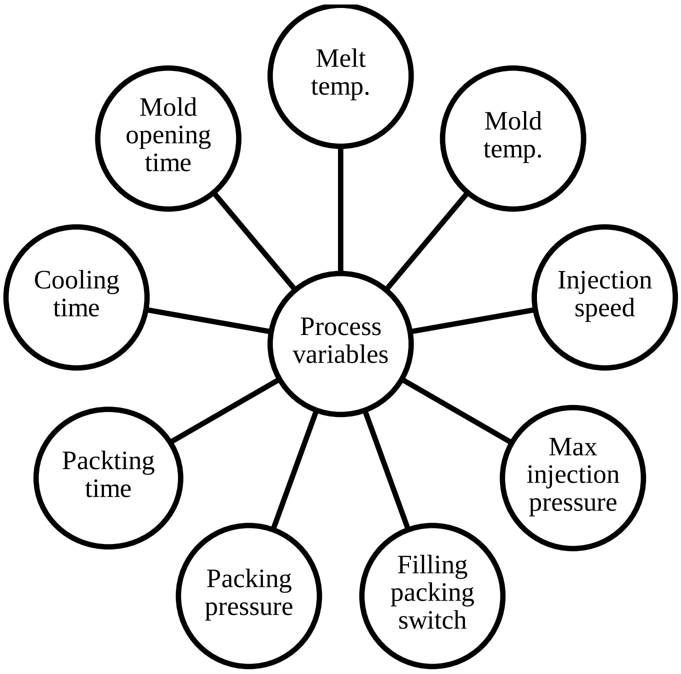

Figure 2.3 Injection molding parameters diagram

There are many injection molding parameters that must be considered and investigated. These factors then bring about the main problem in injection molding, for instance, shrinkage, warpage, cracking, dimensional inconsistency, flashing and short shots.

Indeed, the flow behavior of molten plastic is not only dependent on injection molding parameters, such as melt temperature, mold temperature, injection speed and injection pressure, but also on other parameters which are shear rate and viscosity. The change in each parameter has its own effects on other parameters. Hence, the study of the injection molding factors and the controlling become very complicated.

2.3 Rheology of polylactic acid [7]

The term “rheology” refers to the study of deformation and flow of matter. The term “viscosity” mentions to the resistance of a fluid while it deforms under shear stress. These two terms are directly related in meaning. Hence the rheology of polymer is very useful for explaining the flow behavior of PLA in filling stage of injection molding process.

The viscosity behavior of molten PLA can be extremely complicated. So the melt flow indices (MFI) are created to clarify the viscosity manners of polymer. Unfortunately, the MFI is a single point approximation of the viscosity, which indicates that MFI is not a good representative of the characteristic of the selected material because it cannot cover a broad range of shear rates, temperatures and the pressures when it is being molded. As a result, the various viscosity models have been developed for plastic injection molding.

For example, the Cross-Williams–Landel–Ferry (Cross-WLF) can be used as a capable model of the melt viscosity of Non-Newtonian fluid, η, as a function of shear rate, $\dot{\gamma}$, temperature, T, and pressure, P. To describe the non-Newtonian behavior, a Cross WLF model is employed as expressed in Equation 2.1.

$$\eta(\dot{\gamma}, T, P) = \frac{\eta_0(T,P)}{1+\left(\frac{\eta_0\dot{\gamma}}{\tau^*}\right)^{1-n}} \tag{2.1}$$

In this model, η_0 is the Newtonian limit in which the viscosity approaches a constant at very low shear rates, τ^* is a critical stress level at which the viscosity transitions from the Newtonian limit to power law regime, and n is the power law index in the high shear rate regime. The expression of the Cross model is promptly comprehensible since these three parameters, η_0 , τ^* and n, can be estimated directly from a log-log plot of the viscosity as a function of shear rate as shown in Figure 2.4.

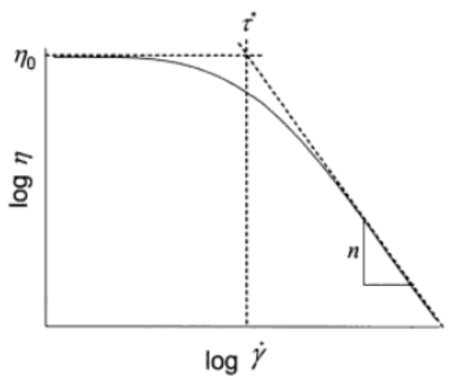

Figure 2.4 Cross-WLF model terms

From Equation 2.1, the zero shear viscosity , η_0 is a function of temperature, T, and pressure, P. The temperature dependence can take many forms, but one of the most common forms uses WLF temperature dependence which includes pressure dependence through the shifting of the glass transition temperature, τ^* which is shown as follows.

$$\eta_0(\mathrm{T,P}) = \mathrm{D_1}\exp\left(-\frac{\mathrm{A_1(T-T^*)}}{\mathrm{A_2+(T-T^*)}}\right) \qquad \mathrm{T} > T^* \tag{2.2}$$

$$\mathrm{T^*(P)} = D_2 + D_3P \tag{2.3}$$

$$\mathrm{A_2} = \tilde{A}_2 + D_3P \tag{2.4}$$

The data-fitted coefficients, $n, \tau^*, D_1, D_2, D_3, A_1$ and $\tilde{A}_2$ are usually determined by curve fitting experiment shear-viscosity data taking by a capillary rheometer at shear rates from 10 to 10,000 1/s. The material properties and Cross-WLF constants for many thousands types of plastics have been fortunately characterized in open source references. The data-fitted coefficients of PLA 7000D is expressed by the following table.

Table 2.1 Cross-WLF model constants for the PLA 7000D used in simulation [8]

Symbol	Value	Unit
n	0.25	-
τ^*	$1.00861\text{x}10^5$	Pa
D_1	$3.31719\text{x}10^9$	Pa.s
D_2	373.15	K
D_3	0	K/Pa
A_1	20.194	-
$\tilde{A}_2$	51.6	K

From Table 2.1, the pressure dependence term in Cross-WLF can be neglected in this work because Cross-WLF model constant, D3, is equal to zero which takes the last term in Eqn. 2.3 and 2.4 equal to zero, too.

Nonetheless, the most important necessity of viscosity model that are employed to express the interested flow behavior of the common melted polymer could reach the subsequent requirements [9]:

- In terms of viscosity and temperature relationship:
  1) The viscosity should decrease with increasing temperature.
  2) The curvature of the iso-shear rate curves should be such that the viscosity decreased at a decreasing rate with increasing temperature.
  3) The iso-shear rate curves should never cross over.
- In terms of viscosity and shear rate relationship:
  1) The viscosity should decrease with increasing shear rate.
  2) The curvature of the isotherms should be such that the viscosity decreases at a decreasing rate with increasing shear rate.
  3) The isotherms should never cross over.

2.4 Plastic flow characteristic [10]

2.4.1 Fountain flow

Fountain flow is normally used to describe how the molten plastic is filling to the mold cavity in plastic injection molding process. Generally, the molten plastic in the center of the cross section moves at the highest velocity. When a molecule of plastic at the center of the cross section reaches to the flow advancement or flow front, it tracks the flow front to the mold wall inside the mold cavity, sticks to it, cools and turns to a frozen layer. Particularly, the primary molecules are directly injected into the mold cavity originate the outer most layer, whereas the latter molecules enter to the center of the mold cavity which is displayed in Figure 2.5

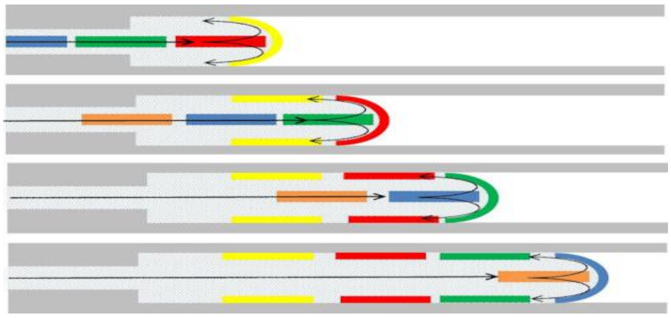

Figure 2.5 Fountain flow [11]

2.4.2 Cross-sectional flow and molecular orientation

In general, there are many the considerable variations in the cross section of the mold cavity e.g. molecular direction, shear rate and shear stress distribution. Shear rate is employed as how fast one molecule is sliding past the other molecules or the difference in velocity over distance which is measured in units of 1/s. Shear stress is force over an area with units of pressure. During filling stage, the plastic molecules in the center of the plastic flow advancement are creeping at a high but relatively consistent velocity. Hence, the shear rate is low and the little shearing tensile force will be appeared on the molecules. Although the velocity is too low around the solidified layer, this velocity has the significant velocity gradient which makes the shear rate increase simultaneously. This situation also generates the high shear stress on the plastic molecules which will stretch or align the molecules in the flow direction as presented in Figure 2.6

Figure 2.6 Molecular orientation through the cross section [12]

2.4.3 Cross sectional heat transfer

Due to the high shear rate involved especially near the solidified layer, there is an important amount of heat buildup with the cross section. The center of the flow channel brings fresh hot plastic material from the plastic injection machine. The mold temperature is relatively cold when comparing with the plastic. When the plastic enters to the mold and touches the mold wall it sticks, cools, and solidifies. The thickness of the solidified layer sustains rapidly as long as the flow rate is still steady. During filling stage, most of the heat transfer is from the high shear zone just inside the frozen layer. Especially while the mold cavity is being filled, the amount of heat extracted into the mold is equal to the heat generated by shear as clarified in Figure 2.7

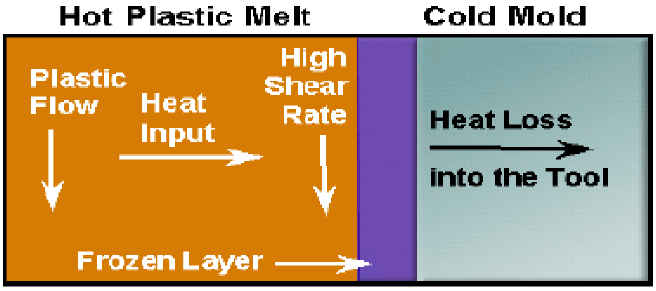

Figure 2.7 Heat transfer in the cross section

2.4.4 Injection rate and frozen layer thickness

The injection rate or injection velocity has an important effect on the thickness of the frozen layer during filling stage. While the mold is being filled the amount of shear heat generated is dependent on the filling rate. The higher the filling rate or the shorter the filling time, the more shear heat that is generated and the thinner the frozen layer will be. The slower the injection rate, the thicker the frozen layer. When the frozen layer gets thicker, the actual flow channel for the plastic gets smaller requiring a higher pressure for a specified flow rate. The opposite is true when the frozen layer gets thinner.

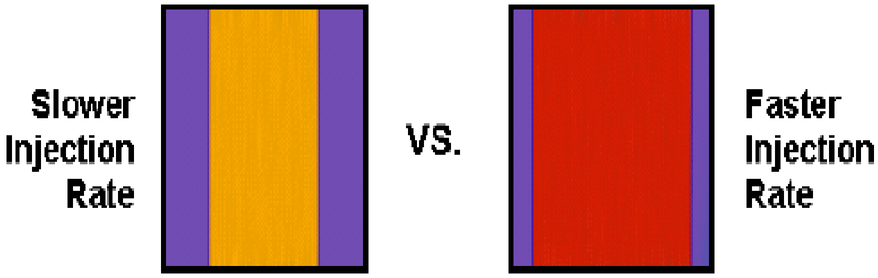

Figure 2.8 Injection rate effect on the frozen thickness

2.5 Computational Fluid Dynamics (CFD)

Computational fluid dynamics is abbreviated as CFD which is used as a computer based calculation for simulating and predicting the fluid flow behavior. CFD consists of 3 basic fundamentals which are mathematics, engineering fluid dynamics and computer science. The various industries that related the fluid dynamics count on this simulator such as automotive, aerospace and chemical industries. Currently, there are many developers expand the commercial CFD packages such as CFX, FLUENT, STAR-CD, CFD-ACE, PHONICS and FLOW3D. In this research, CFX package is utilized.

2.5.1 The history of CFD

The CFD is used as commercial software in 1980s. The commercial CFD was on the basis of very complicated non-linear mathematical expressions that specify the elementary equations of fluid flow, heat and mass transfer. Due to the complex computer algorithms set in CFD are used to solve these equations iteratively and numerically. Thus, the effective computer is required for CFD solvers. Luckily, the high performance computer in the present can decrease the time and cost in modeling and analyzing of CFD. Therefore, the CFD is now a new design tool in the industries because it not only reduces the design timescale but also enhances industrial process.

2.5.2 CFD solution procedure [13]

There are 3 main inner-connectivity stages within a CFD analysis framework, namely pre-processing stage, solver stage and post-processing stage. The details of each element are examined as follows.

● **Pre-processing stage**

The pre-processing stage is used as the problem setup step which can be divided into 4 steps as shown in Figure 2.9.

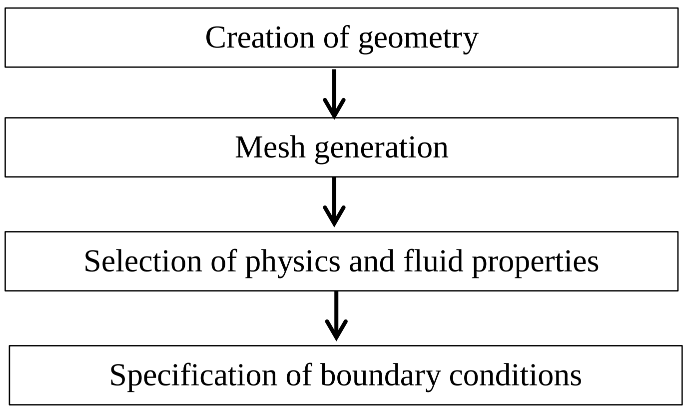

Figure 2.9 Steps in pre-processing stage

In general, the purpose of the first step in pre-processing stage is to define and create the geometry of the flow region. The geometry of flow region and domain are performed so as to prepare the inputs for the mesh generation. The mesh generation is used to divide the domain into the smaller cells or control volumes and then the fluids that are expressed as these cells are usually solved numerically. So this represents one of the most important steps during the pre-processing stage after the specification of the domain geometry. Since, the accuracy of a CFD solution is governed by the number of cells in the mesh domain. In selection of physics and fluid properties part, the user has to identify the appropriate flow physics in order to correctly simulate the characteristics of the fluid flow. Lastly, a CFD user needs to specify the boundary conditions to make the simulation model closed to the actual process as much as possible.

● **Solver stage**

The CFD solver resolves governing equations together with the rheological characteristic of the selected material by using Cartesian spatial coordinates and velocity components. The governing equations consist of mass, momentum and energy balance equations as shown in Equations 2.5, 2.6 and 2.7, respectively.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0 \tag{2.5}$$

Equation 2.5 is the mass conservation equation and is valid for incompressible and compressible flows. The conservation of linear momentum is explained by as follow:

$$\frac{\partial (\rho U)}{\partial t} + \nabla \cdot (\rho U \otimes U) = -\nabla p + \nabla \cdot \tau + S_M \tag{2.6}$$

Where, p is the absolute pressure, S_M is momentum source and the stress tensor τ is related to the strain rate by following equation:

$$\tau = \mu(\nabla U + (\nabla U)^T - \frac{2}{3}\delta \nabla \cdot U) \tag{2.7}$$

Instead of conservation of energy equation, the thermal energy is used to take into consideration the viscous dissipation of the polymer melt during mold filling. The thermal energy equation is:

$$\frac{\partial (\rho h_{tot})}{\partial t} - \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U h_{tot}) = \nabla \cdot (\lambda \nabla T) + \nabla \cdot (U \cdot \tau) + U \cdot S_M + S_E \tag{2.8}$$

Where h_{tot} is the total enthalpy that is related to the static enthalpy $h(T, p)$ by:

$$h_{tot} = h + \frac{1}{2} U^2 \tag{2.9}$$

The term $\nabla \cdot (U \cdot \tau)$ represents the work due to viscous stresses and is called the viscous work term and represents $U \cdot S_M$ the work due to external momentum.

Initially, the mold cavity is assumed to be filled fully by air and the polymer melt is injected the air in the cavity out of mold during plastic injection molding. To model this fluid flow problem, a multiphase approach with the surrounding air and melted polymer as the two phases flow is employed. The transport equations which are continuity equation and linear momentum equation are transformed to be the multiphase approach. The continuity equation is:

$$\frac{\partial}{\partial t}(r_\alpha \rho_\alpha) + \nabla \cdot (r_\alpha \rho_\alpha U_\alpha) = S_{MS\alpha} + \sum_{\beta=1}^{N_p} \Gamma_{\alpha\beta} \tag{2.10}$$

Where the $S_{MS\alpha}$ describes user specified mass sources and the $\Gamma_{\alpha\beta}$ is the mass flow rate per unit volume from phase β to phase α. This term only occurs if interphase mass transfer takes place. The multiphase linear momentum equation is:

$$\frac{\partial}{\partial t}(r_\alpha \rho_\alpha U_\alpha) + \nabla \cdot \left(r_\alpha(\rho_\alpha U_\alpha \otimes U_\alpha)\right) = -r_\alpha \nabla p_\alpha + \nabla \cdot \left(r_\alpha \mu_\alpha (\nabla U_\alpha + (\nabla U_\alpha)^T)\right)$$

$$+ \sum_{\beta=1}^{N_p} \left(\Gamma_{\alpha\beta}^{+} U_\beta - \Gamma_{\beta\alpha}^{+} U_\alpha\right) + S_{M\alpha} + M_\alpha \tag{2.11}$$

Where $S_{M\alpha}$ describes momentum sources due to external body forces, and user defined momentum source. The M_α represents the interfacial forces acting on phase due to the presence of other phases. The $\Gamma_{\alpha\beta}^{+} U_\beta - \Gamma_{\beta\alpha}^{+} U_\alpha$ is the momentum transfer induced by interphase mass transfer.

In this study, a transient simulation is chosen for simulating the filling stage in injection molding process of melted polymer. To model the free surface flow problem of the melted polymer at every time step, the volume of fluid (VOF) or volume conservation equation is applied for melt front tracking. The volume of fluid is expressed by the following transport equation:

$$\sum_\alpha \frac{1}{p_\alpha}\left(\frac{\partial p_\alpha}{\partial t} + \nabla \cdot (\mathrm{r}_\alpha \mathrm{p}_\alpha \mathrm{U}_\alpha)\right) = \sum_\alpha \frac{1}{p_\alpha}\left(S_{MS\alpha} + \sum_{\beta=1}^{N_p} \Gamma_{\alpha\beta}\right) \tag{2.12}$$

The VOF method is created by means of the important assumption that all phases are supposed as a continuous phase which means that all field variables are treated to be shared between the phases. This modeling approach usually uses a phase indicator function, or it may be called color function, to track the interface between two or more phases. The indicator function has value one or zero when a control volume is entirely filled with one of the phases and a value between one and zero if an interface is occurred in the control volume. Thus, the phase indicator function has the properties of volume fraction [14].

So as to solve these equations, the finite volume method is applied as a standard numerical solution technique to convert all of these equations to algebra equations and consequently solve these algebra equations numerically.

● Post-processing stage

CFD has a prestige of creating realistic graphics image and, while some of them are promotional and are usually presented in stunning and great colorful outputs. The ability to display the simulation results effectively in as invaluable design tool. In this part, some essential computer graphic techniques are frequently concentrated encountered in the presentation of CFD data. The CFD results are emphasized graphically and can be classified under different categories. It can assist the CFD user to better analyze and visualize the many relevant physical characteristics within the fluid flow problem.

2.6 Mesh topologies [15]

The one important function in CFD simulation program is meshing. ANSYS CFX Meshing is used to separate the whole domain into several control volume elements. There are 2 main categories of meshing which are 2 dimensional (2D) and 3 dimensional (3D) meshes. For 2D meshes, for example quadrilateral and triangular elements are applied for the surface meshing. In contrast, the 3D meshes namely hexahedral, tetrahedral, pyramid, wedge, and polyhedral cells can be used for volume meshing. These all structured meshes, as well as hybrid meshes consisting quadrilateral and triangular cells or hexahedral, tetrahedral, pyramid, and wedge cells are acceptable for applying in ANSYS CFX as displayed in Figure 2.10.

In summary, choosing the mesh type depends on application, simulation or computational time. Generally, the mesh type recommended criteria are the triangle and tetrahedron are suitable for the cumbersome domain because theirs structure can handle with the complex sections of the domain. Conversely, the quadrilateral and hexahedral cells are relatively appropriate for the simple structures since the common domain can be divided within the smaller control volumes when comparing with the triangle and tetrahedron.

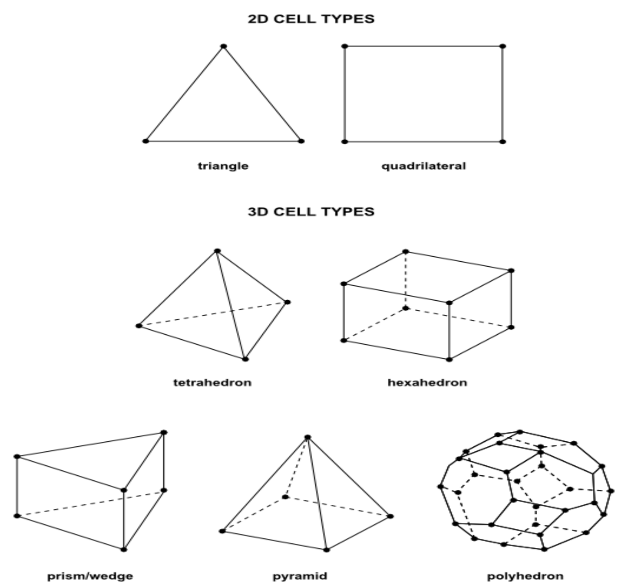

Figure 2.10 Types of cell [16]

2.7 Literature review

Galantucci L.M. and Spina R. [4], 2003, suggested an integrated numerical simulation to determine gating system configuration to optimize the filling conditions of thermoplastic molded part. The finite element (FE) analysis and design of experiment approach (DOE) were used in this study. In sum, the FE was suitable for investigating stress and strain distributions in filling, post-filling and cooling phases of injection molding process. Nonetheless, this procedure was sensitive to the differences between property of material and geometry of mold.

Gan et al. [17], 2010, proposed the mold filling analysis of polystyrene by using finite volume method in order to predict the precise filling time which can prevent the molding defects. In this study, the polystyrene was modeled as non- Newtonian, non-isothermal and compressible fluid dynamic problem. This problem was solved by using computational fluid dynamic package, ANSYS CFX, together with continuity, conservation of linear momentum and thermal energy equations. The non-Newtonian behavior was described by a viscosity model, Cross WLF. In order to verify the numerical predictions obtained from finite volume method. The simulation results from finite volume method were compared with the injection molding simulation software results, MoldFlow. It was found that these results were compatible but the filling time of ANSYS CFX was 0.14s longer than MoldFlow prediction. Moreover, the effect of process variables on mold filling was analyzed by using different melt temperatures and mass flow rates. It can be concluded that the melt temperature showed more significant effect on pressure along the melt flow length. The shear stress decreased with temperature, in contrast, shear stress increased with mass flow rate.

Khor et al. [18], 2010, presented the three-dimensional numerical and experimental investigations on rheology in meso-scale injection mold of ABS plastic. In this literature, the mold filling analysis is simulated by Gambit and FLUENT 6.3 software with Cross-Arrhenius for viscosity model. They observed that the suitable temperature and shear rate ranges for injection molding were 200-260 ºC and 10^2 -10^4 s^{-1} respectively which were agreed with previous researchers. Furthermore, the compared results between simulation and experiment were in good line, which indicated that the FLUENT 6.3 can handle with injection molding problem.

J. Koszkul and J. Nabialek [19], 2007, investigated the methods of modeling of polymer injection molding in exiting process of polycarbonate with glass fiber. This study was carried on by comparing the simulation results from Moldflow Plastics Insight 6.1 (MPI) with the results of video recording for plastic flow in real process. The simulation software was solved together with the viscosity model, Cross-WLF. In conclusion, the simulation software can deal with the composite plastic injection molding process problem and gives the satisfactory results as well.

Tsung-Lung WU [20], 2008, presented a 3D numerical simulation of biodegradable polymeric scaffold of tissue engineering on precision injection molding. The plastic material of scaffold is used for PLA material. The experiment was separated into 3 levels involving the 4 different injection molding parameters and values, namely mold temperature, melted temperature, injection pressure and packing time. The Taguchi method was used to find the optimum condition for biodegradable injection molding. In sum, the results from Moldflow Plastics Insight (MPI) showed that the temperature, pressure and shear stress distribution were uniform which implied that the warpage phenomenon cannot happen. However, this study found that the main problems of PLA plastic can occur like degradation, short shot and flash. The results showed the melt temperature was larger than 230 ºC and injection pressure was larger than 50 MPa, the degradation situation of PLA was formed. In contrast the melt temperature was lower than 190 ºC and injection pressure was larger than 12.5 MPa, the short shot event was occurred. Lastly, this inferred that the optimum condition, melt temperature 210 ºC and injection pressure 20 MPa, was also determined by Taguchi method.

Chuan-zhen Qi et al. [21], 2012, studied the effect of the injection compression molding (ICM) parameters, such as the melt temperature, injection speed, mold temperature, compression distance, and compression speed. The experiment showed that the most important factor that causes the warpage was melt temperature. And the effect order of the parameters from the simulation analysis was melt temperature, injection speed, mold temperature, compression distance and compression speed, respectively.